undamental capabilities in Science, Technology and Engineering are an ever-more critical foundation of our nation's prosperity and security. We are in a new unstable global environment, and it will be essential for Sandia to provide solutions to the nation's most press-



ing problems. The challenges are too complex to be solved by linear extensions of our existing knowledge and too urgent to await the serendipity of the usual innovation process. As in the past, meeting these challenges requires extensive strategic partnering with the university and industrial communities and, when appropriate, other government agencies and institutions. Add a sense of urgency as catastrophic weapons and measures fall into the hands of terrorists."

Pace VanDevender

Vice President Science, Technology, and Engineering

Making Over-the-horizon Concepts Real

A strong science, technology, and engineering heritage extends into the future

The confluence of hypothesis and unparalleled experimental facilities has been augmented by still-growing computational capabilities in many areas but especially in modeling/simulation. Sandia's traditional science and engineering

Mary Crawford tests the output of an ultraviolet lightemitting diode developed by a team that set new records for wavelength/power output.

processes are accelerated by ever-more powerful computing capabilities; so too are our computing capabilities strengthened and refined as we progress and tackle larger problems.

Wars for domination of the world plagued civilization for nearly 4,000 years until 1945, followed by the decades-long Cold War. Today, the threats to the nation's security and well-being are far different but equally dangerous. The science, technology and engineering programs at Sandia remain rooted in our primary mission as stewards of the nuclear deterrent to wars of global domination. We are committed to producing advances of the same magnitude to end the newer scourge of terrorism, with fundamental benefits for the nation and the world. These order of magnitudes advances occur across the spectrum of science and engineering. They may involve single scientific steps that work their way up to revolutionize whole processes, or they may be large, engineered systems with a worldwide impact. Increasingly, they are computed solutions for previously intractable problems.

Our Grand Challenges inspire our scientists and engineers to make real concepts that are currently over the horizon of today's technologies. These challenges, in fields as diverse as atmospheric studies, energetic materials, nuclear and fusion energy, and reliability studies, attract new talent and partnerships across the nation.

The impressive technical achievements of miniaturization and integration in the MicroChemLab™ demonstrate the cross-lab coordination that will occur

in the future Microsystems and Engineering Sciences Applications (MESA) complex. Production of the integrated MicroChemLab™ advances the concept of integrated microsystems by demonstrating how microscale components can be fabricated together into a single silicon chip. The state of the art of high pressure liquid chromotography was substantially advanced through a recent CRADA with Waters Corporation.

Sandia has also signed an Umbrella CRA-DA with HP's Imaging and Printing Group (IPG), one of HP's four business groups. IPG includes printer hardware, digital imaging devices such as cameras and scanners, associated supplies, and accessories. Their business involves many of the same technologies that are core to Sandia, including microfluidics, chemistry, materials science, and photonics. The CRADA will directly benefit Sandia's homeland security and defense missions.



IPG hopes to leverage Sandia technologies to develop new business markets in the life sciences arena, in particular health sensing solutions, to develop new products in display devices/technologies.

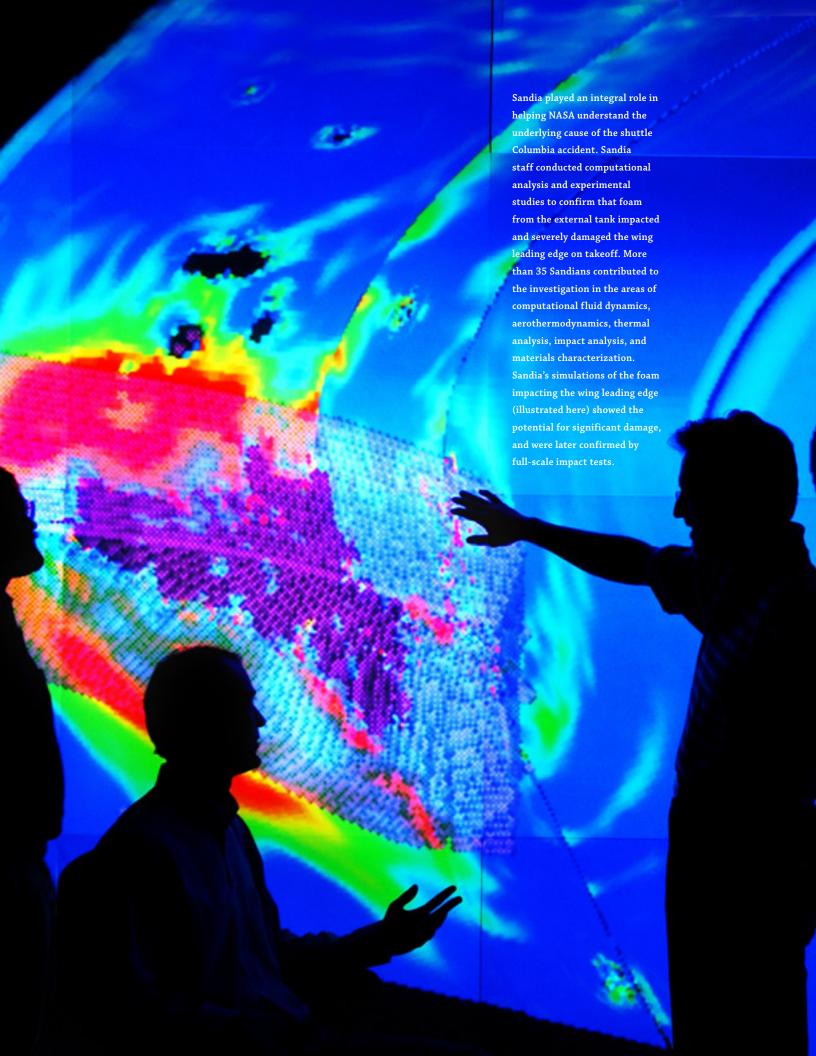
Technological advances in national security—the province of chemistry, physics and mechanical engineering for most of the 20th century—now occur at a far more complex and, obversely, fundamental level. For example, to build robust microsystems, Sandia scientists and engineers soon recognized that nanoscale phenomena came into play, and had to be understood



Front side (a) of monolithically integrated MicroChemLab™ compared to a U.S. dime. Etching visible on the back (b) defines fluidic channels, release holes, and the spiral gas chromatograph column.



Nanotechnologies at Sandia will be developed at a new facility, the Center for Integrated Nanotechnologies, or CINT, in a joint program with Los Alamos National Laboratory. CINT will have four areas of expertise: photonics lattices and quantum clusters; complex, self-assembling nanostructures; the mechanics of behavior at the nanoscale; and importation of biological principals and functions into nano- and microsystems.



and exploited. Nanotechnology, in turn, required an understanding of the ways biological creations assemble and disassemble. More than ever, multidisciplinary and cross-disciplinary research will be critical to generating new insights and discoveries occurring at scientific boundaries. Following are just a few highlights from recent work at Sandia.

Understanding fundamental phenomena

Fundamental work in material sciences resolved a long-standing mystery of how the centuries-old process of annealing metals works. Annealing removes damage and defects from a shaped piece of metal, leaving tough, ductile, perfect crystals behind. Using advanced computer models, Sandia researchers performed the first full-physics simulations of a shaped aluminum substructure. They found that one in a million tiny, pre-existing crystallites grows quickly and large, supplying the nucleus for recrystallization into a cellular structure. These observations provide the basis for a new, physically based understanding of this pervasive metallurgical process.

The researchers also discovered that the cell models, when plotted to a mathematical curve, compare to patterns in the expanding universe. The team is now applying their results to annealing in aircraft aluminum and automotive steel. More realistic annealing models can help industries cut costly time and prototypes from their design schedules. Eventually, engineers may use these models to control sheet metal forming in factories around the world.

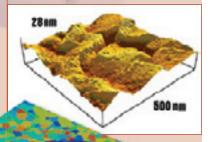
Understanding corrosion is fundamental to understanding why materials fail. We have adopted a novel approach using engineered defects and newly developed analytical techniques to unravel the mysteries of how localized corrosion initiates in aluminum. We are generating mechanistic information by comparing the characteristics of nanometer-length scale degradation processes

scale degradation processes in synthesized protective oxide structures with those in actual alloy systems. This knowledge is critical to developing predictive models of materials aging.

Quantum computing, which uses phenomena at the quantum level of physics, could eventually replace today's digital computing. The innovative materials used in these systems are so pure that the electrons remember their phase over distances of up to 100 microns. Thus they behave more like waves than like particles, and can exhibit wave interference effects, anticrossings of energy levels, and novel collective effects where the positions of individual electrons become correlated with their neighbors to form ordered, collective states.

Another fundamental discovery could lead to revolutionary quantum computing devices with logic, storage, and wiring elements that actually build themselves. Stress in mixed silicon/germanium films, grown under precisely controlled conditions, causes the spontaneous formation of remarkable nanoscale quantum dot molecules in square fortress-like shapes with highly uniform sizes. Furthermore,

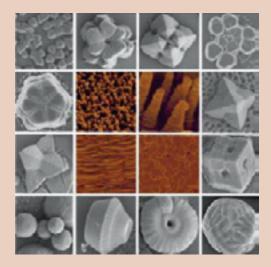
Understanding aluminum film corrosion with an atomic force micrograph.



The universe in a bent piece of metal. In a computer simulation, a few crystalline cells (dark blue) grow at the expense of their neighbors as annealing begins. When annealing is over, the substructure will be entirely consumed. The small cells in this picture are about one-fiftieth the diameter of a human hair. Their spacing pattern compares with that of expanding galaxies following the Big Bang.

Bio-inspired diatomlike and seashell-like zinc oxide (brown) and silicate (gray) crystals.

a focused ion beam can selectively seed the self-assembly process, demonstrating the potential to create complex nanoscale circuits exactly where wanted.



We have devised a general, environmentally benign, chemical-synthesis approach to build complex nanostructures that are strikingly similar to those observed in biominerals (seashells and diatoms). The key to this new approach is to control nucleation and growth events and crystalline surface chemistry. We hope this new class of nanomaterials will lead not only to applications in microdevices, sensing, energy storage and conversion, and catalysis, but will also add to our understanding of how complex biomaterials are formed.

Biological advances fight terrorism and infant leukemia

At the biological interface, motor proteins are molecular machines that enable many materials-assembly and actuation functions in living organisms, including cell division, transport of subcellular structures, and muscle contraction. Sandia is exploring the use of these active proteins to assemble and reconfigure nanomaterials

in artificial systems. As a first step toward creating programmable nanomaterials, we have demonstrated that the motor protein kinesin can transport inorganic materials such as gold nanoparticles and quantum dots in lithographically patterned microfluidic channels.

Sandia scientists, working with the University of New Mexico Cancer Center, have made a significant advance in the understanding of the molecular biology of infant leukemia. By using specialized machine learning techniques, they studied and classified a large collection of microarray data of infant leukemia tissues into three distinct categories. The first two categories, environmental exposure and viral exposure in utero, were expected. However, they showed that there was another category, whose genetic markers indicated a strong correlation with abnormal stem-cell activity. This was a completely unexpected result, and the complete classification of the different types of cancers is an important step toward developing treatments tailored to an individual. This work has led to numerous patents and more importantly, has led to a large number of collaborations around the country in the field of microarray analysis.

Computational capabilities merge modeling/simulation with traditional science methodology

Our computational programs include the building of the 40-teraops (40 trillion operations/second) Red Storm computer; the secure and ultra-fast networking needed for collaboration within Sandia and with other labs; the visualization systems to help comprehend vast data sets, and inno-

vative and powerful software to fully use this computational power to solve real-life problems. These programs are creating and deploying the new architectures required to double computational capabilities every two years. In California we dedicated the Distributed Information Systems Laboratory, which will enable classified and unclassified local and distant collaboration, and significantly reduce development times.

Supercomputing is revolutionizing the way we approach science, and engineer and manufacture all kinds of products. Sandia's contributions, recognized by three Gordon Bell awards—the highest computer science award—are integrating the traditional theory-and-experiment methodology with high-performance computational modeling/simulation to accelerate technical progress. An example of how these enhanced computing facilities help our nation is a Memorandum of Understanding between DOE and the Environmental Protection Agency (EPA) that established an EPA-funded effort focused on leveraging Sandia capabilities to advance the biological, environmental, and computational sciences for EPA's missions. EPA will benefit from Sandia's capabilities for resolving remote sensing and gene expression array data and for speeding-up EPA's Computational Model of Air Quality.

Biotechnology for understanding and bettering quality of life includes national security

Our biotechnology programs are developing basic science and technology for understanding biological processes and harnessing these processes for national

security applications. At our California Hongyou Fan observes

security applications. At our California site, researchers have made significant and unique contributions to the science of structural proteomics. Starting from a bare-wall 'bio' capability a little over three years ago, they are unraveling the complexities of membrane protein structures. This positions Sandia to play an important role in defense against biowarfare agents, particularly as protein-based receptors can be tuned to detect specific toxic molecules.

fluorescence by nanocrystals in water solution. The dark vial holds gold nanocrystals; the orange and green vials are semiconductor nanocrystals.

Work is under way to identify and learn how to exploit key strategies used by living systems to develop materials whose assembly and disassembly can be programmed or self-directed. This may lead to new nanomaterials that can be programmed for assembly, reconfigura-

New materials for environmental extremes

As weapon systems advance and material performance requirements are pushed to extremes, we must develop new materials to match these environmental extremes. In many cases, components can survive

Sandia's Red Storm computer was under construction in late 2004.





Sandia's \$37.9-million
Distributed Information
Systems Laboratory in
California will enable development and deployment
of new technologies for the
nuclear weapons complex.
The lab is a critical element
in a strategy to develop and
deploy high-performance
modeling and simulation
capabilities.

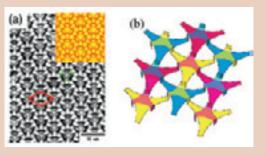
tion, healing, and disassembly. Just as the ability to direct and bound processing on the microscale via semiconductor lithography has enabled scores of electronic advancements, the ability to pattern and direct biochemically relevant molecules will open new horizons in engineering at the molecular scale.

The successful demonstration of multilevel patterning of DNA, phospholipids, proteins, and cells has been the first step toward achieving this molecular scale organization. This work supports sensor designs ultimately based upon single molecular responses. only if the environmental loads can be shared with a secondary, synergistic structure. Some highlights:

- We developed new materials with exceptional toughness that absorb energy from extreme environments and distribute impact forces broadly, preventing catastrophic failures in new weapon applications.
- We have made significant improvements in ultra-high-temperature ceramics for use in advanced thermal protection systems. These materials melt above 3,200°C and are strong and resistant

to thermal shock. These materials are needed to manage the 2,000°C temperatures expected from atmospheric heating of maneuverable, hypersonic vehicles that are proposed for a number of defense, surveillance, and space missions.

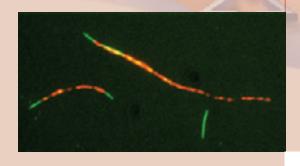
■ Electronic and mechanical parts often contain interfaces between dissimilar materials. These interfaces often crucially affect overall materials strength of a part. We have discovered a new structure for these interfaces, with perfect metal on both sides separated by a single layer of specially arranged metal atoms. This structure promises to provide an extremely strong shear-resistant bond.



(a) An experimental scanning tunneling microscope image of the nanoscale dislocation array with a theoretical (yellow) simulation of the structure. (b) A schematic of the perfect array of nanoscale dislocations that are interwoven to lock the two bulk metals together.

■ Friction and wear are major concerns in the performance and reliability of micromechanical (MEMS) devices.

While many friction-reducing materials are available, it is difficult to apply uniform coatings to the intricate three-dimensional (3-D) structures typical of MEMS devices. We have developed a novel coating process, called atomic layer deposition, which uniformly coats



shadowed surfaces, such as gear hubs and teeth with wear-resistant or lubricating films.

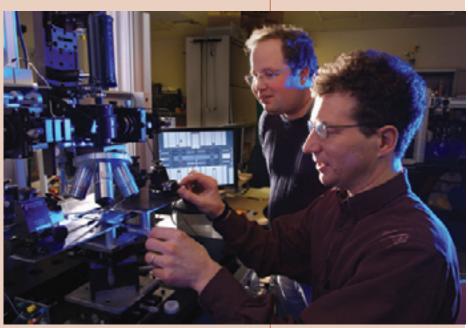
New technologies in photonics and electronics for lighting efficiency, fighting terrorism

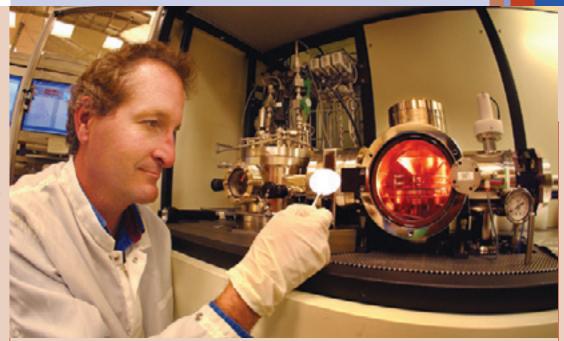
In past research, Sandia's photonic lattice showed the ability to bend light with no loss of efficiency. Now a microscopic tungsten lattice—a filament fabricated with an internal crystalline pattern—has the potential to transmute infrared energy into the frequencies of visible light. This would raise the efficiency of an incandescent electric bulb from five percent to greater than 60 percent, greatly reduce the need



A simplification of a self-assembled monolayer containing the motor protein kinesin propelling a microtubule shuttle carrying nanoparticle "cargo." The image is from a fluorescence microscope movie of the transport by kinesin of quantum dots.

Martin de Boer (right) and Alex Corwin investigate friction at the microscale.





Andy Allerman is growing new UV LED materials that operate at shorter wavelengths, making it possible to build miniaturized devices that can detect biological agents, perform covert communications, purify water, cure polymers and other chemicals, and decontaminate equipment.

for excess electrical generating capacity, and reduce the costs of electrical lighting. The advance also opens the possibility of increased efficiencies in thermal photovoltaic applications.

Our breakthrough in deep ultraviolet solid-state, light emitting diodes (LEDs) has led to large increases in output. These LEDs have been used in demonstrations of bio-agent detection and a non-line-of-sight communication system. Further development could enable water purification, decontamination, and thin-film curing.

decontamination, and thin-film curing.

With the Massachusetts Institute of Technology, we have achieved world-record long-wavelength lasing from quantum cascade lasers. We have generated wavelengths as long as 141 microns (frequency >2 TeraHz) and record operating temperatures in this regime (137K pulsed and 93K continuous operation). TeraHz spectroscopy has potential for rapidly identifying chemical and biological agents and for imaging applications. Sandia is one of only three laboratories worldwide that has demonstrated the sophisticated compound semiconductor growth required for these structures.

Z Machine produces first confirmed fusion neutrons

We continue to leverage Sandia's and other leading institutions' expertise and successes in pulsed power, high energy density physics, and material dynamics for the nation's pressing issues in weapon science, thermonuclear fusion energy, and national security applications of high-power and high-power/density beams.

Inertial confinement fusion (ICF) capsule implosions in the Z machine have produced the first clearly measured neutrons

Each crystal for terahertz lasers takes approximately 17 hours to grow in a 175step process on this 10foot-long, seven-foot-high, molecular beam epitaxy machine.

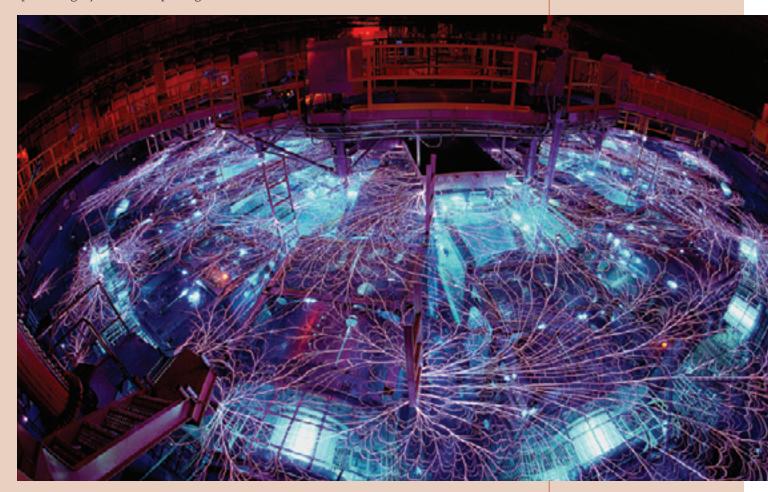
and X-ray images of imploded fuel symmetry. We confirmed that deuterium fuel reached temperatures found at the center of the sun (about 11 million degrees C.). Capsules have been imploded to less than 1/2000 of their original volume, implying a radiation-drive symmetry that scales to within approximately a factor of two of high-yield fusion requirements. Uniform 3-D compression is an essential step in creating controlled nuclear fusion.

We completed a unique concept for using Z-pinch fusion technology to generate electrical power. Using advanced manufacturing technology, critical components are remanufactured every 10 seconds to support a high-yield fusion pulse generated

by a driver based on Sandia's Z accelerator technology. This radically different, yet simpler, approach to fusion energy will compete with other fusion concepts.

A Sandia team, with assistance from Ktech and Bechtel, has developed a containment system that can shocklessly compress materials to greater than 1.5 million atmospheres of pressure (one-third the pressure at the center of the earth) using Z, then hermetically seal the chamber in 10 microseconds. Six shots have demonstrated the system's reliability to contain hazardous materials, including highly radioactive ones. This system enables revolutionary dynamic materials studies.

Sandia's Z pulsed-power generator, the most powerful X-ray generator on Earth, has become nationally recognized for dynamic materials research.



Nickel Brand Software in
Moriarty helps bridge the
gap between historical
(hot iron branding) and
current animal identification methods. Working
with the Space Alliance
Technology Outreach
Program, Sandia has demonstrated a recognition
software that is compatible with scanners and
hand-held computers for
ease-of-use on the range.



The Cumbres & Toltec narrow gauge steam railroad remains a major tourist attraction in Northern New Mexico long after its working life would otherwise be over. Recently Sandia researchers helped the Cumbres & Toltec repair shop with some critical metallurgical analysis. The railroaders needed to know the composition and other properties of certain metals before doing any welding for restoration and repairs.

Sandia Supports Innovative Small Businesses

The New Mexico Small Business Assistance program allows Sandia to use a portion of its gross receipts taxes paid each year to provide technical advice and assistance to small businesses in the state. During 2003, Sandia received \$1,796,000 million in tax credits, 64 percent of which went to small businesses in rural New Mexico and 36 percent to small businesses in Bernalillo County, where Sandia's main facility is located. Technologies and technical assistance come from virtually all areas of Sandia's expertise. Following are some examples of this assistance:

■ Applied Thermal Systems and Beer Engineering perform research and development in the areas of systems engineering, complex robotics, automation systems, networks, and software development. Sandia's assistance has provided the two companies valuable experience with the capabilities and limitations of commercially available robots through work on a pick-and-place robotic work cell project.



- Enterpulse, Inc. is a research and development company in pulsed power specializing in automotive ignition, specifically spark plugs. Sandia assisted in the development of a new spark plug that has the potential to be 10,000 times more powerful than current spark plugs. This assistance allowed Enterpulse to overcome a major hurdle in development and expedited the fabrication process.
- Fast Ditch™ in Vallecito is in the commercialization stage of producing a unique corrugated plastic liner for earthen ditches to reduce the loss of water that occurs with unlined ditches. Based on burn testing provided by Sandia, new liners will be designed to minimize the surface area of the ditch that is exposed to weed burning.

■ Last Chance Water Company in Otero County is a water management company representing landowners of the Salt Basin. The company manages water resources and establishes the water supply available to potential markets. Sandia is assisting in the identification, quantification, and characterization of a new and renewable water source within the state.



- New Mexico Chile Taskforce in southern New Mexico is a partnership of chile growers, producers, and researchers created to apply science and technology to improving productivity and ultimately enhance New Mexico growers' competitiveness in a global market. Sandia has provided a remote system to evaluate efficiency of automated chile cleaning and destemming machines now under development.
- **PEMCO** in Farmington is one of only five companies in the United States that provides repair and refurbishment services for well drilling and servicing rigs. Partnering with NM Manufacturing Extension Partnership, Sandia has helped PEMCO meet current industry standards and requirements for management and manufacturing practices and techniques. That translates to about \$150,000 in annual cost savings.
- STAR Cryoelectronics in Santa Fe develops, manufactures, and markets ultra-sensitive Superconducting Quantum Interference Device (SQUID) sensors and advanced PC-based SQUID control electronics products worldwide. With Sandia's assistance the company modified a process and eliminated defects that were causing device failures.

Sandia also provided assistance through the Small Business and the Mentor Protégé program to 12 of the 40 start-up companies included in this year's *Albuquerque Journal's* Flying Forty—an annual list of New Mexico firms producing the most revenue or greatest revenue growth. The companies include: Emcore, Ktech, CVI Laser, Holman's, Optical Insights, TMC Design, MesoSystems Technology, Team Specialty Products, Optomec, Stolar Horizon, Management Sciences, and TPL.

Partnering for a Strong America

Sandia's industry and university partnerships are key to our mission of providing cost-effective scientific and engineering solutions to meet national needs in nuclear weapons and related defense systems, homeland security, energy security, and environmental integrity—and to address emerging national challenges for both government and industry.

Since its inception in the early '90s, Sandia has executed more than 580 CRADAs, 930 non-federal entity agreements, 940 commercial licenses to Sandia-developed intellectual property, and more than 2,800 small business assistances.

CRADAs and other types of Partnering

Umbrella CRADAs continue to be the preferred contractual instrument for implementing strategic and enduring relationships. At least 15 such agreements have been executed with industrial partners and recently Sandia signed CRADAs with Toyota, FM Global, Catalytic Distillation Technologies, and American Superconductor Corporation.

Sandia's relationship with Lockheed Martin, the Shared Vision program, serves as a model for strategic partnerships. This highly successful collaboration is applying technologies and systems developed by both organizations to the challenging defense and security threats of our changing world. Shared Vision projects in microelectronics and photonics, sensors, situation and decision support modeling,

cognition, nanotechnology, biotechnology, anti-tamper devices, and logistics support have offered applications for both government and industry.

Award-winning partnerships

The R&D 100 Awards, which annually recognize significant advances in technology, are a measure of Sandia's success in developing technologies that impact the nation's security and prosperity. Since the award's inception, Sandia has won 70 R&D 100 awards. This year, Sandia was involved with two award-winning technologies.

One award is for a new process of growing gallium nitride on an etched sapphire substrate, called cantilever epitaxy, which promises to make brighter green, blue, and white LEDs—solid state lighting. The cantilever epitaxy program at Sandia was part of an internal three-year, \$6.6 million Laboratory Directed Research and Development Grand Challenge. Funding also came from a grant from the DOE Office of Building Technologies for a collaborative project with Lumileds Lighting, a joint venture between Agilent Technologies and Phillips Lighting.

The second award was for the creation of the software framework and library Trilinos. Trilinos is part of a broad effort on the part of national laboratories, industry, and academia to establish high-fidelity computational modeling and simulation as an approach to engineering and scientific understanding so it becomes an equal partner with the most basic approaches of theory and experiment. Trilinos provides a common enabling solution to one of the most difficult problems in creating

Christine Mitchell looks through a substrate that was made for the new cantilever epitaxy growth process.



these simulations: How can one solve the massive and complex systems of equations required, and do so in a way that "scales" all the way from laptop computers to the most powerful and complex parallel computers in the world? Trilinos offers what is probably the largest and most complete scalable solver capability in the world, and it is available to the public.

A commitment to university programs

University partnerships are a critical element in achieving the goal of making Sandia the laboratory that the U.S. turns to first for technology solutions to the most challenging problems that threaten peace and freedom for the nation and the globe. Sandia has traditionally contracted for university research to expand its science and technology base to assure the performance of its nuclear weapons, but many partnering opportunities exist in other Sandia mission areas.

Today, Sandia partners with key universities to achieve three major objectives: conduct world-class science, hire world-class scientists and engineers, and develop strategic collaborations in focused research areas. In Fiscal Year 2003, Sandia invested about \$21 million in joint research projects with universities. We worked with 109 universities and had about 500 active contracts with them. Sandia also devotes about \$15 million a year for graduate student support and university and science outreach.

Two Massachusetts Institute of Technology postdoctoral students have been selected as the first recipients of the President Harry



S. Truman Research Fellowship in National Security Science and Engineering at Sandia. Truman Fellowship candidates are expected to have solved a major scientific or engineering problem in their thesis work or have provided a new approach or insight to a major problem, as evidenced by a recognized impact in their field.

The Sandia Campus Executive Program provides a framework for Sandia to focus our research goals and helps us create the 21st-century workforce needed to perform the technical jobs crucial to fulfilling our national security mission. Sandia executives, acting in the role of ambassadors, are paired with top university officials (usually deans of engineering) at schools that have synergistic research interests and capabilities with Sandia. The campus executives and their teams visit their assigned universities once or twice each



year, serve on university advisory boards, and attend special events. They actively support placing students in the numerous Sandia programs. Sandia partners with universities on numerous research projects, some also involving other government or industrial partners.

25,457-square-foot building, Innovation Center, in the park.

■ Sandia's SS&TP program office won both a Sandia Employee Recognition Award and a Gold President's Quality Award for mangement of the park.

Since its inception in 1998, the SS&T Park has been widely recognized as a model for public/private partnerships around the country.



Sandia Science & Technology Park

The Sandia Science & Technology Park (SS&TP), a 200-acre, technology community located adjacent to the Labs in Albuquerque, continues to grow. Sandia serves as the anchor to the park, offering companies access to scientists, engineers, technologies, and cutting-edge facilities. Among the past year's success stories:

- Ktech Corporation and its 170 employees, a Sandia strategic partner, moved into a new 84,300-square-foot building in the park.
- Sandia's Controller and Pension Plan Management Center moved into a new

- Heel, Inc. opened a new 52,546-squarefoot building, housing corporate offices and production facilities. The firm currently employs 70 people, with growth potential to 150 by 2010.
- New Mexico Senator Pete Domenici spoke at a ceremony marking a major upgrade to the park's fiber optic network. The Department of Commerce's Economic Development Administration presented a check to the park for \$750,000 at the ceremony to purchase networking and switching equipment for the network.